**Surface effects in the (001) BaTiO3 ferroelectric slab from first-principles calculations and phase field simulation**

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We have investigated out-of-plane polarization in the (001) ferroelectric BaTiO3 slab using first-principles and phase-field calculations. In the phase-field simulation, the change of polarization near the surface by the surface relazation effect has been modeled using an extrapolation length. The effects of BaTiO3 slab size, surface terminations (BaO and TiO2 terminated surfaces) and value of extrapolation lengths have been obtained from ab initio calculations on the basis of density functional theory. By combining with phase field simulation based on Landau-Ginzburg theory[1], it was found that the polarization of ferroelectric thin films is dependent fully on the extrapolation length of films.

1. J. Wang, T.Y. Zhang, Phys. Rev. B, 73, 144107 (2006).